

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
 Data File : BF095060.D
 Acq On : 10 May 2017 17:26
 Operator : SJ/MA
 Sample : I3061-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VL-WWTP-002

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.042	353	358	384	rBV	711680	1355145	42.76%	6.125%
2	5.001	512	521	534	rBV	904210	1711504	54.01%	7.736%
3	5.660	630	633	652	rBV	265613	638291	20.14%	2.885%
4	6.207	722	726	739	rBV	291123	396572	12.51%	1.792%
5	7.266	902	906	919	rBV2	129103	337070	10.64%	1.523%
6	7.366	919	923	940	rVB	949332	1456408	45.96%	6.583%
7	7.707	976	981	989	rBV	376794	478983	15.12%	2.165%
8	7.942	1016	1021	1036	rVB	1723327	2022573	63.83%	9.142%
9	8.607	1129	1134	1158	rBV	1140858	1590662	50.20%	7.189%
10	9.730	1321	1325	1342	rBV	387937	581909	18.36%	2.630%
11	11.501	1621	1626	1648	rBV	2456002	3118450	98.41%	14.095%
12	12.201	1741	1745	1755	rBV	95655	140717	4.44%	0.636%
13	12.560	1801	1806	1819	rBV2	493443	734788	23.19%	3.321%
14	13.395	1943	1948	1953	rBV2	36887	45330	1.43%	0.205%
15	13.548	1970	1974	1977	rBV	86754	123334	3.89%	0.557%
16	13.607	1981	1984	1992	rVB2	66111	110173	3.48%	0.498%
17	13.854	2021	2026	2040	rBV	755810	1200621	37.89%	5.427%
18	14.171	2075	2080	2090	rBV	39366	64600	2.04%	0.292%
19	14.901	2201	2204	2209	rVB2	34493	37119	1.17%	0.168%
20	14.959	2209	2214	2227	rVB2	517532	748184	23.61%	3.382%
21	15.324	2272	2276	2281	rVB	38053	42898	1.35%	0.194%
22	15.389	2282	2287	2293	rVV	31878	39828	1.26%	0.180%
23	15.459	2293	2299	2311	rVB2	17030	36757	1.16%	0.166%
24	15.624	2323	2327	2334	rBV	58960	72938	2.30%	0.330%
25	15.924	2375	2378	2385	rBV2	153254	195784	6.18%	0.885%
26	17.012	2557	2563	2576	rBV	97673	158825	5.01%	0.718%
27	17.289	2604	2610	2620	rBV	2580910	3168854	100.00%	14.323%
28	18.541	2819	2823	2833	rBV6	17608	43343	1.37%	0.196%
29	18.630	2833	2838	2853	rVB	573903	767174	24.21%	3.467%
30	20.294	3117	3121	3134	rBV2	343812	534800	16.88%	2.417%
31	20.818	3206	3210	3217	rBV4	35502	60674	1.91%	0.274%
32	20.977	3233	3237	3242	rVB7	24807	36192	1.14%	0.164%
33	21.724	3357	3364	3373	rBV7	23556	74370	2.35%	0.336%

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ALS Vial : 6 Sample Multiplier: 1

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

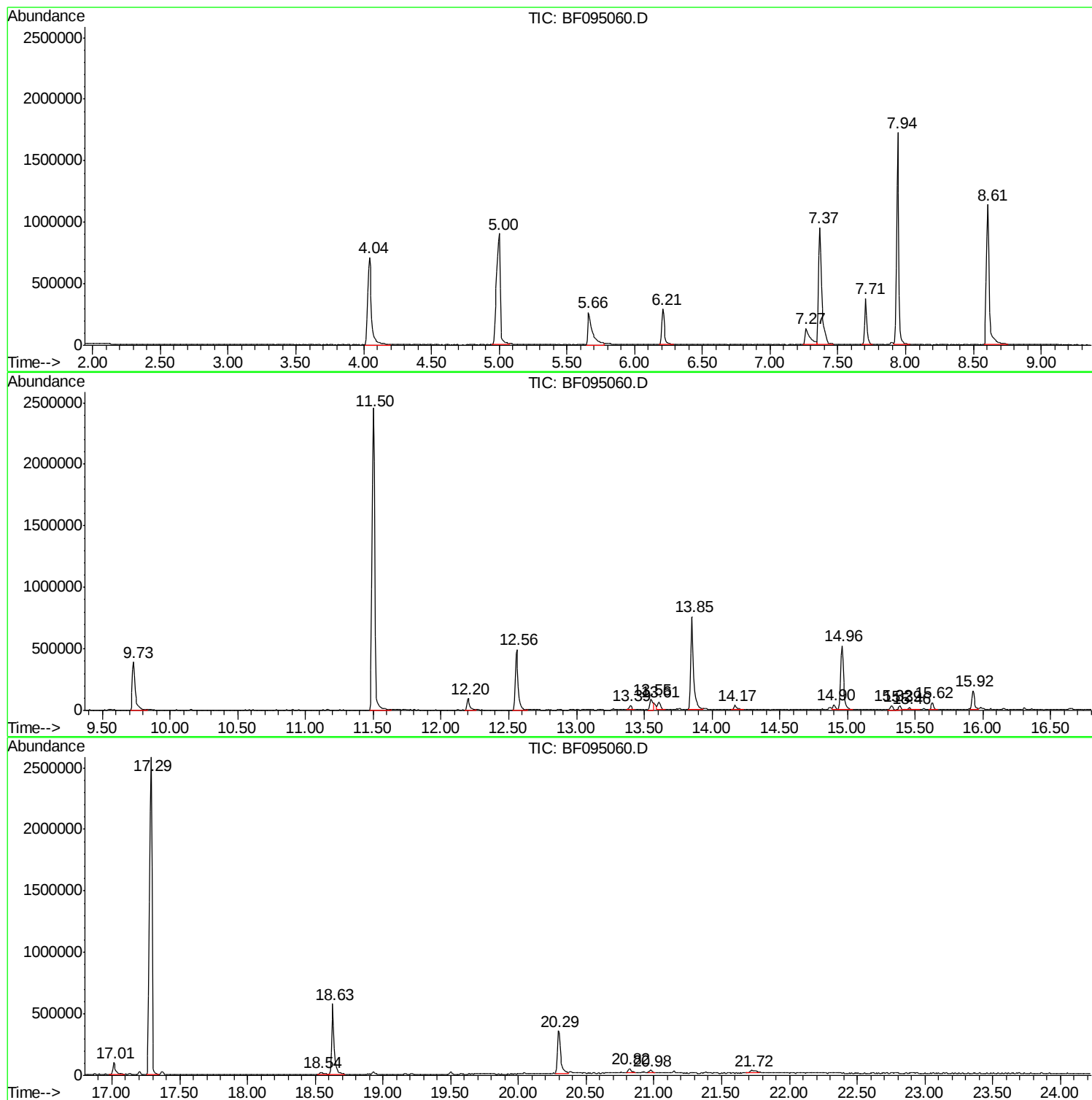
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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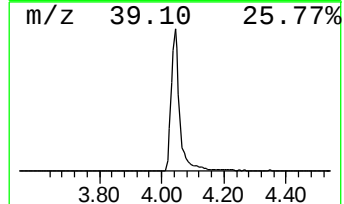
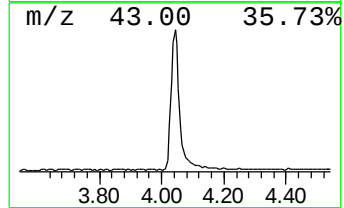
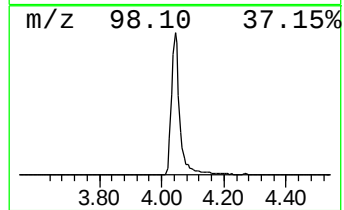
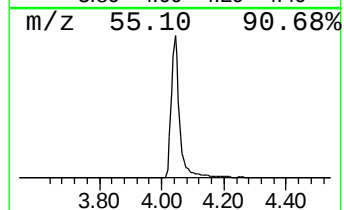
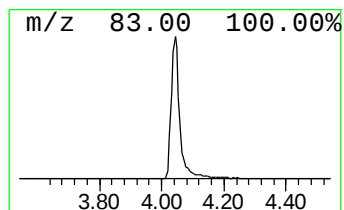
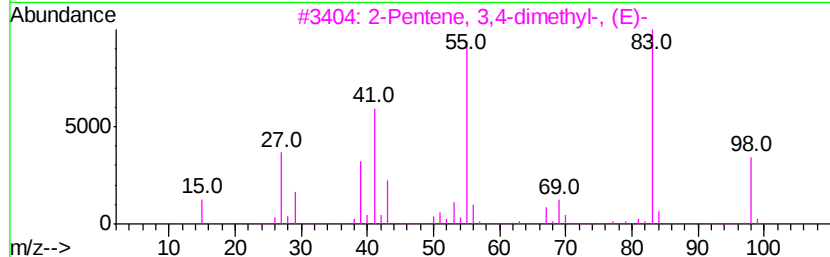
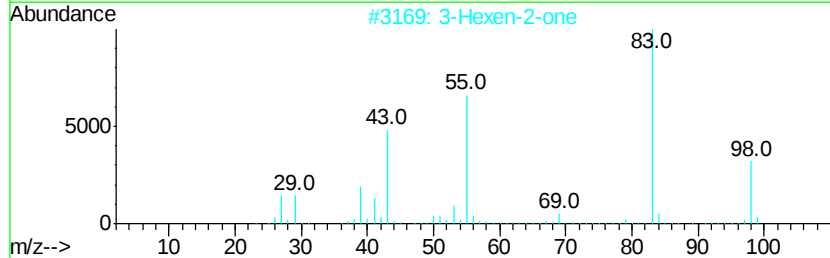
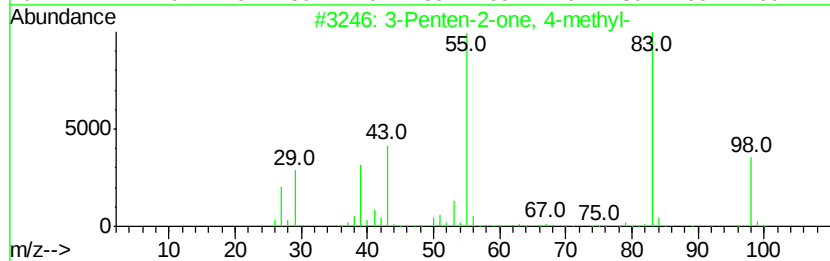
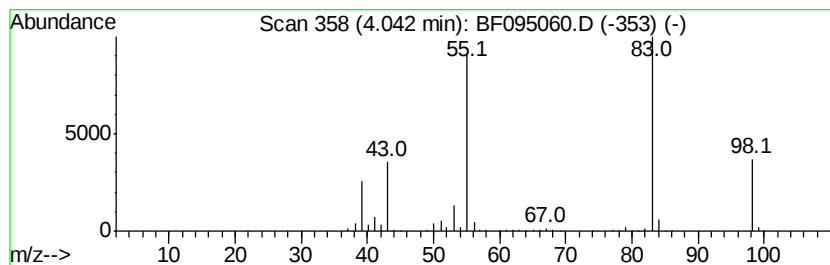
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.04	56.58 ng	1355150	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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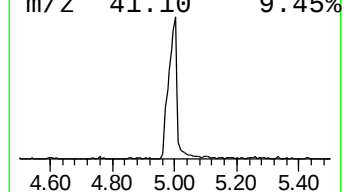
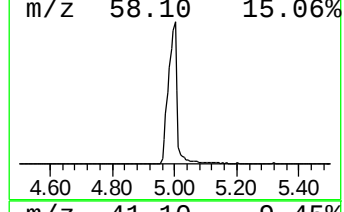
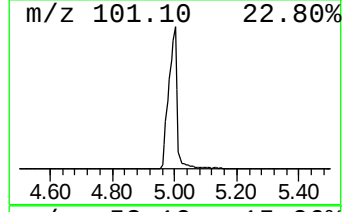
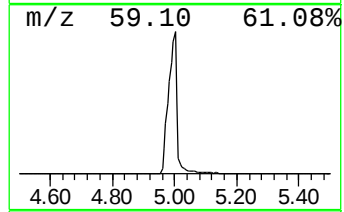
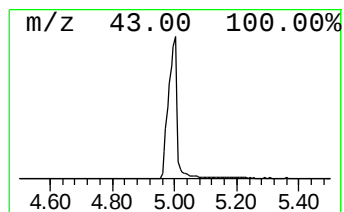
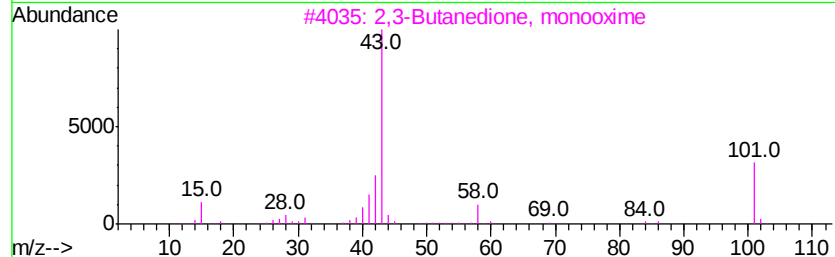
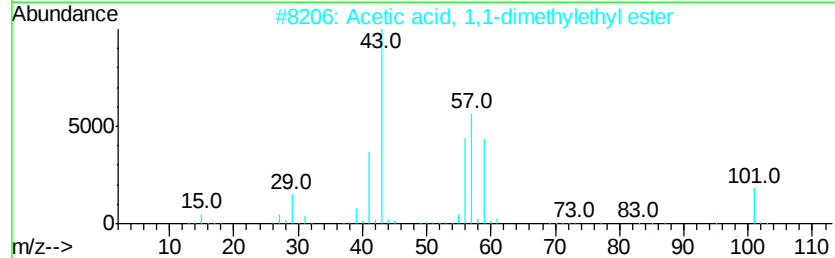
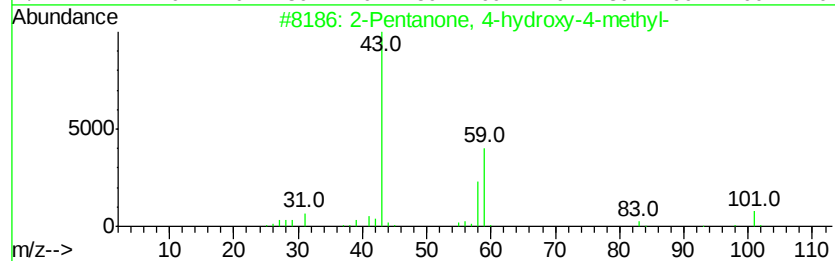
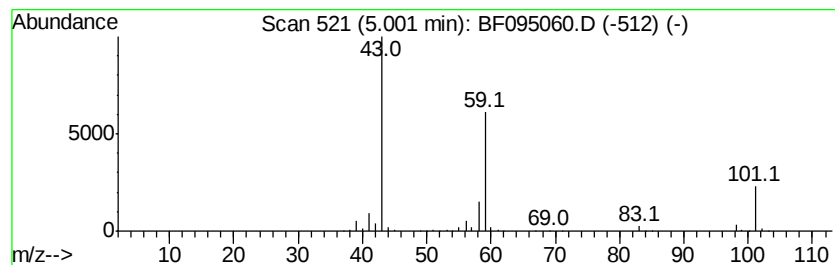
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	71.46 ng	1711500	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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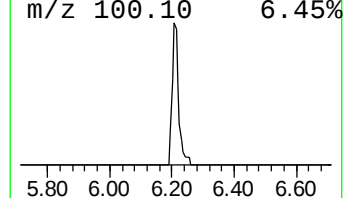
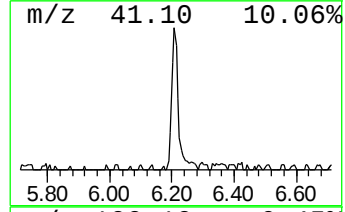
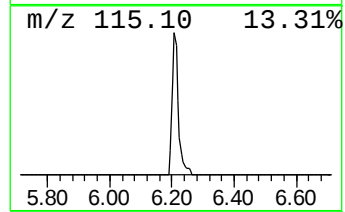
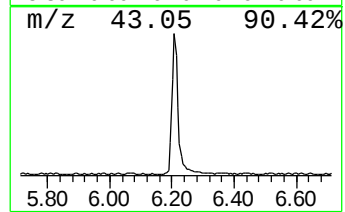
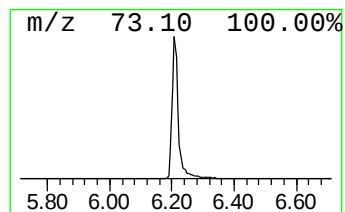
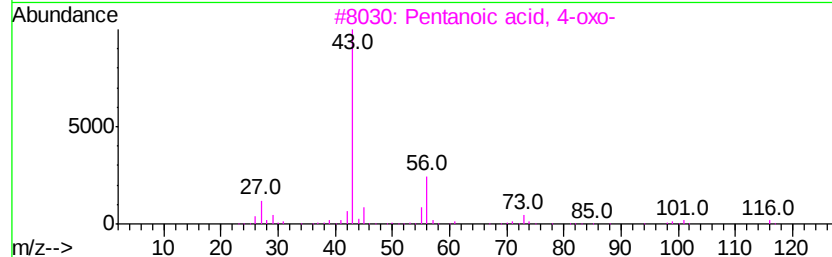
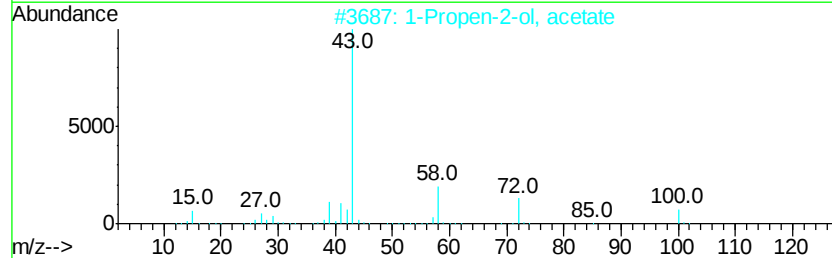
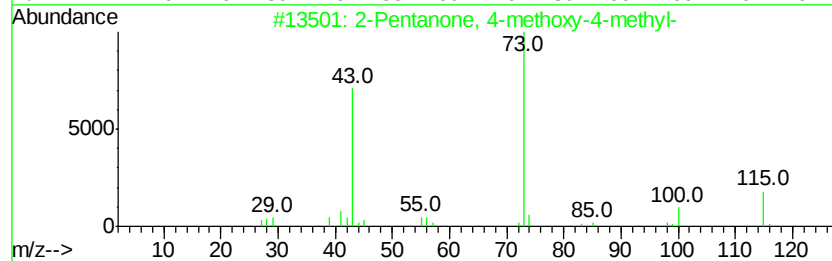
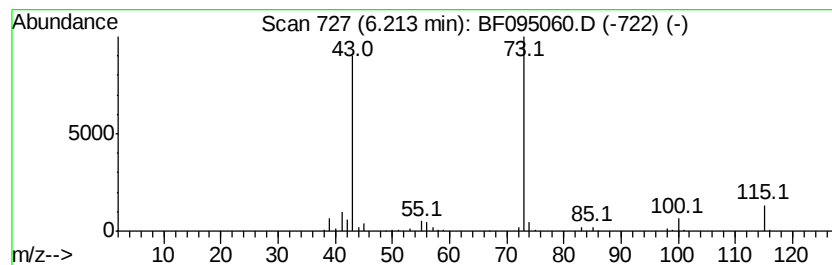
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	16.56 ng	396572	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
3		Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	12
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10



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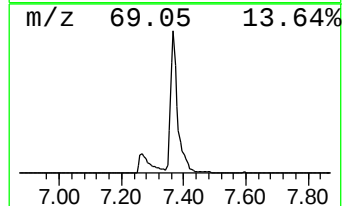
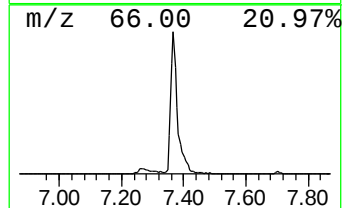
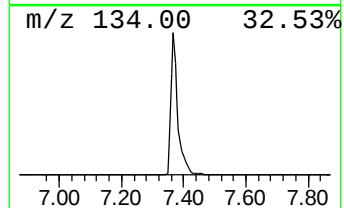
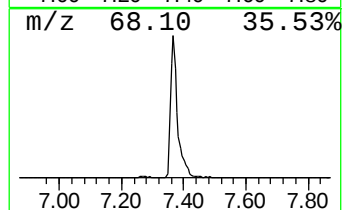
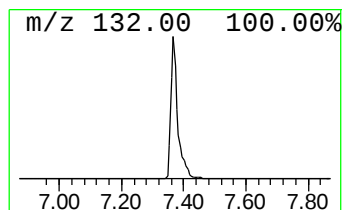
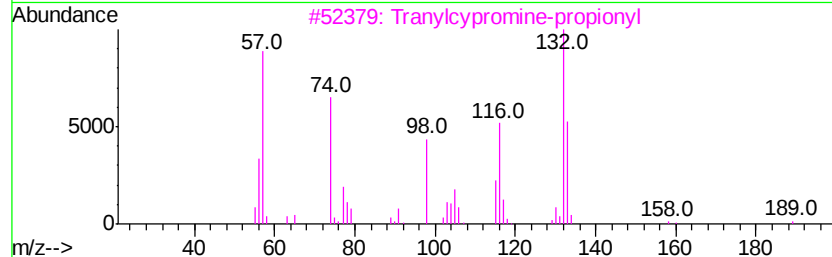
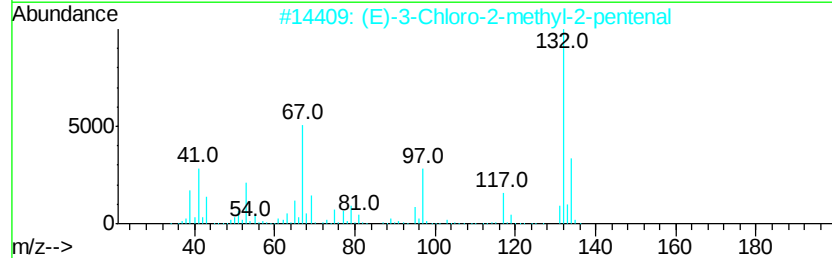
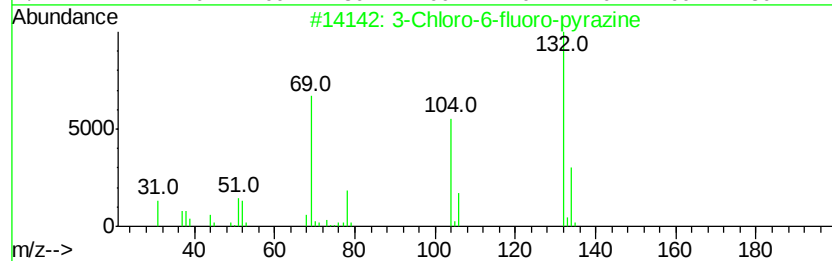
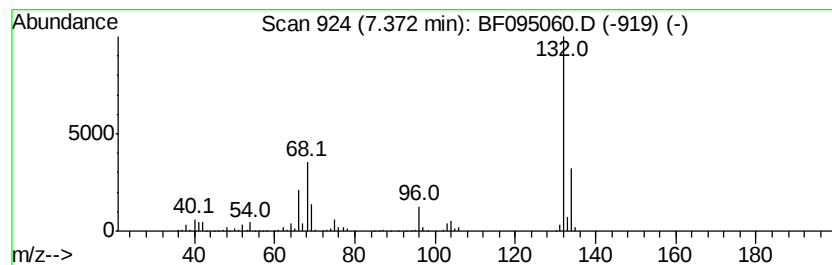
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.37 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	60.81 ng	1456410	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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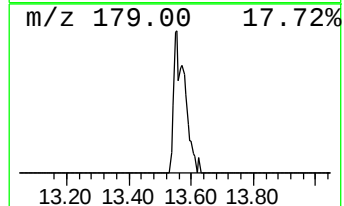
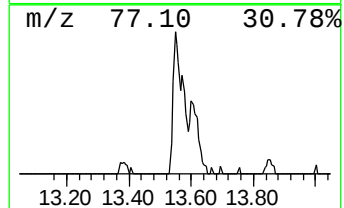
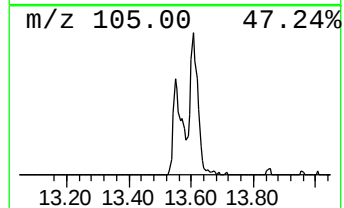
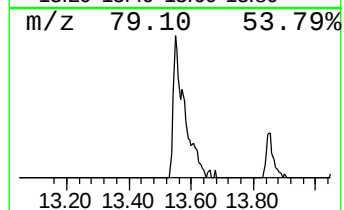
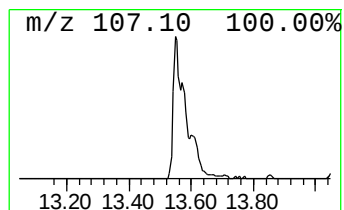
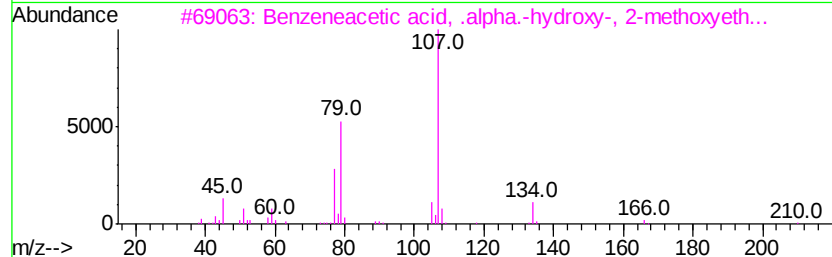
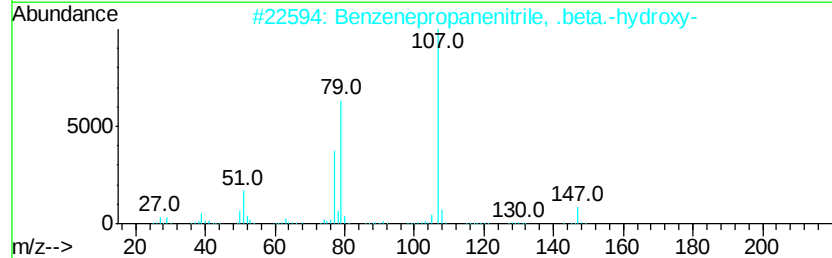
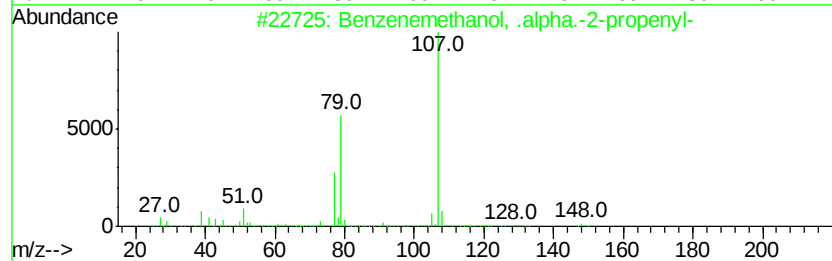
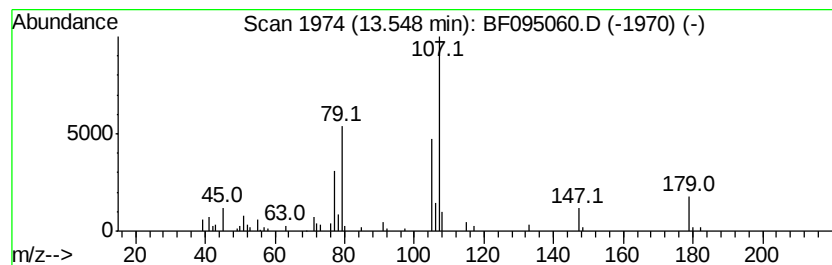
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenemethanol, .alpha.-2-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	3.36 ng	123334	Acenaphthene-d10	12.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanol, .alpha.-2-prope...	148	C10H12O	000936-58-3	72
2		Benzenepropanenitrile, .beta.-hy...	147	C9H9NO	017190-29-3	72
3		Benzeneacetic acid, .alpha.-hvd...	210	C11H14O4	1000221-86-4	64
4		3-Hydroxy-2-methyl-3-phenyl-prop...	180	C10H12O3	1000372-54-5	64
5		Ethyl mandelate	180	C10H12O3	000774-40-3	64



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
Data File : BF095060.D
Acq On : 10 May 2017 17:26
Operator : SJ/MA
Sample : I3061-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VL-WWTP-002

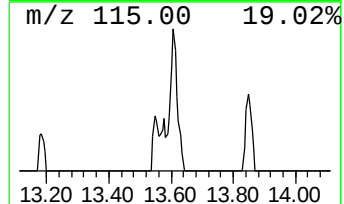
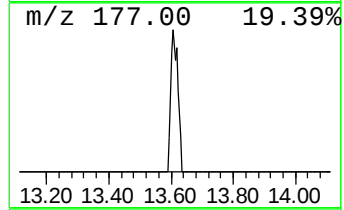
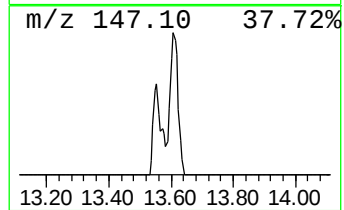
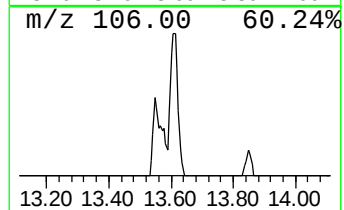
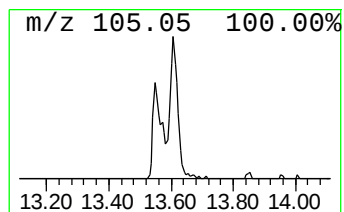
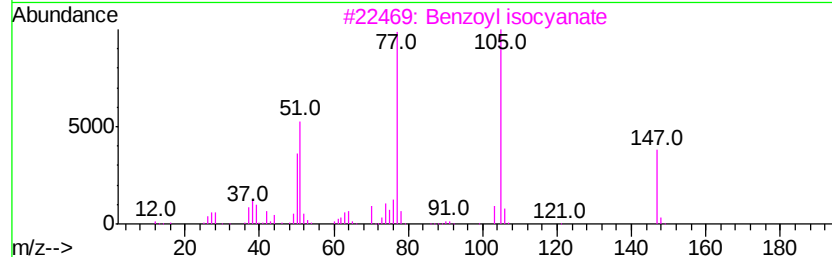
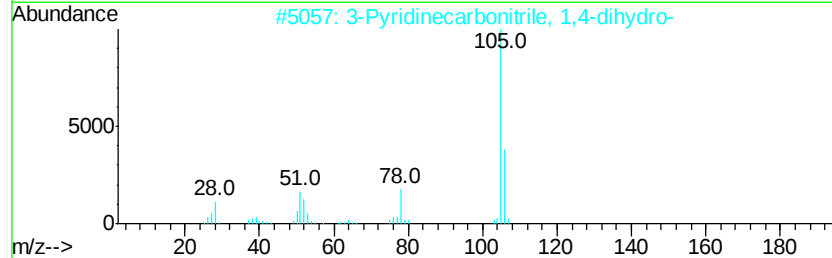
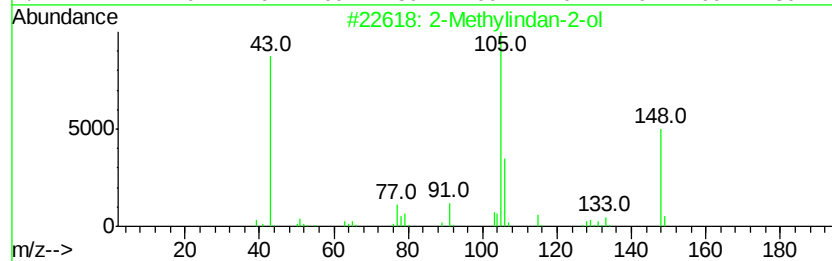
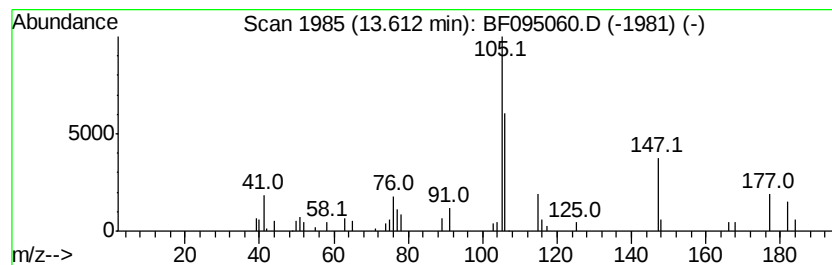
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown13.61 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	3.00 ng	110173	Acenaphthene-d10	12.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindan-2-ol			148	C10H12O	033223-84-6	38
2	3-Pyridinecarbonitrile, 1,4-dihy...			106	C6H6N2	023974-91-6	35
3	Benzoyl isocyanate			147	C8H5NO2	004461-33-0	17
4	Benzoic acid, 3,5-dibromo-4-meth...			439	C17H15Br2NO3	1000258-73-5	10
5	Benzoic acid, 4-hydroxy-3-nitro-...			330	C16H14N2O6	346661-98-1	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
Data File : BF095060.D
Acq On : 10 May 2017 17:26
Operator : SJ/MA
Sample : I3061-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VL-WWTP-002

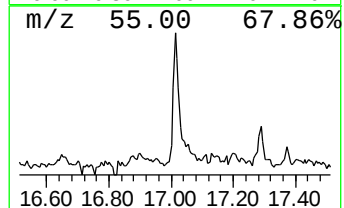
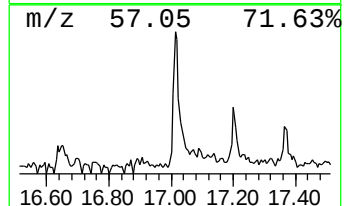
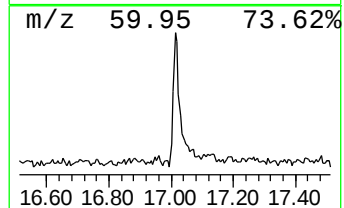
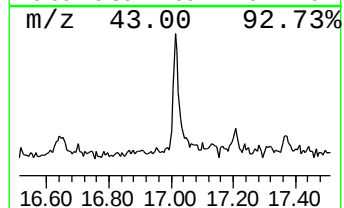
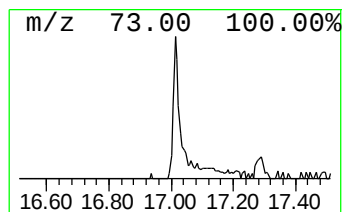
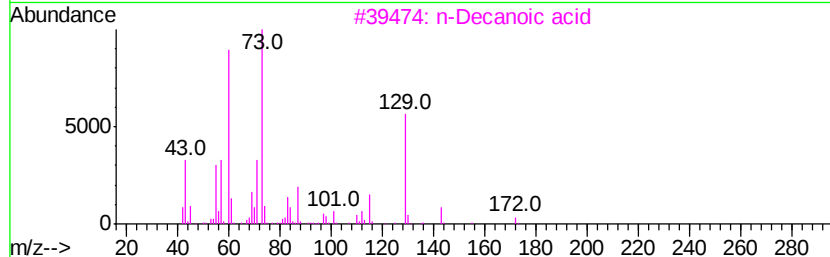
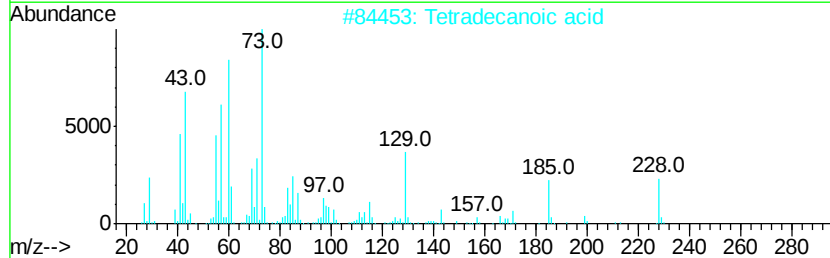
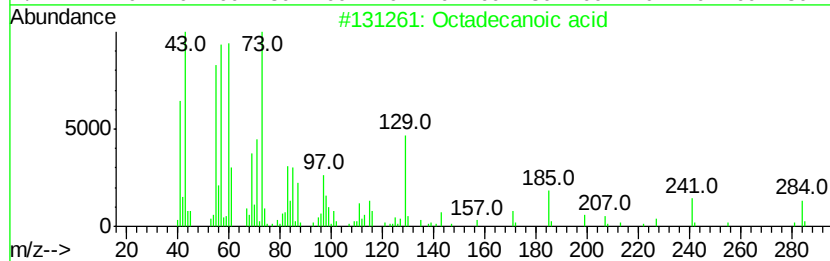
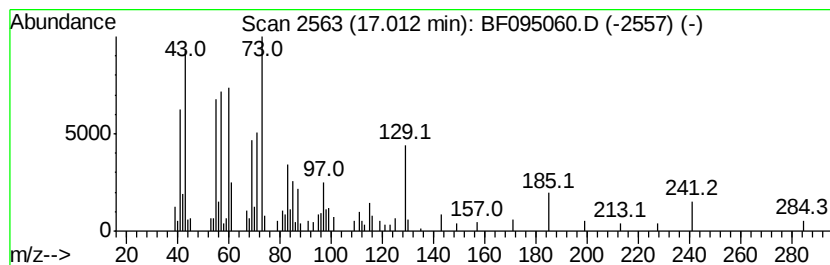
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	4.14 ng	158825	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3		n-Decanoic acid	172	C10H20O2	000334-48-5	52
4		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	11
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	11



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
Data File : BF095060.D
Acq On : 10 May 2017 17:26
Operator : SJ/MA
Sample : I3061-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VL-WWTP-002

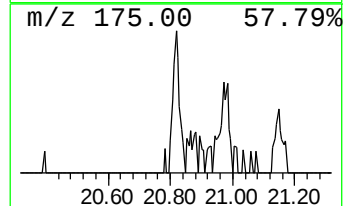
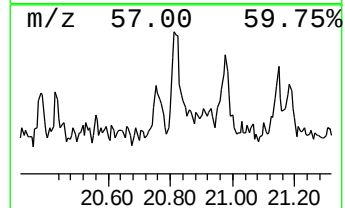
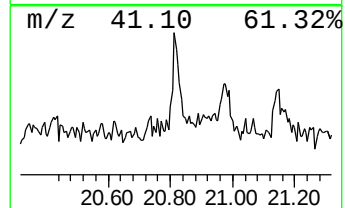
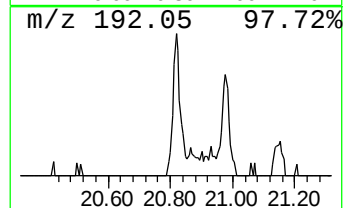
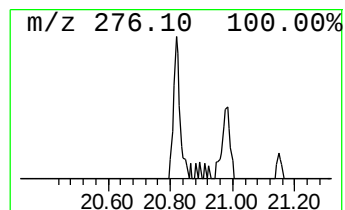
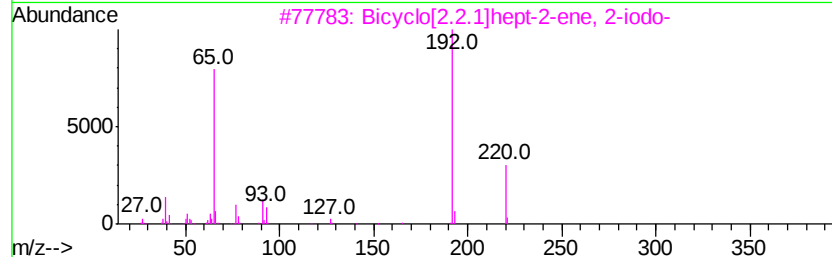
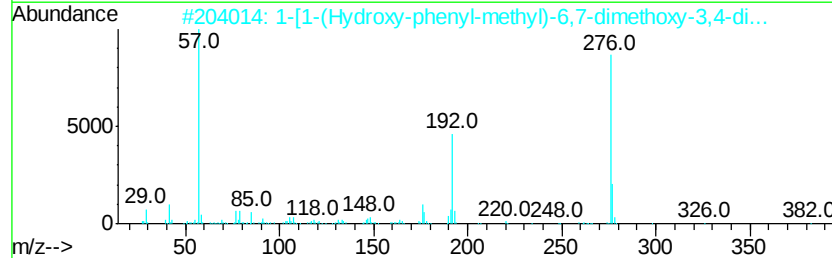
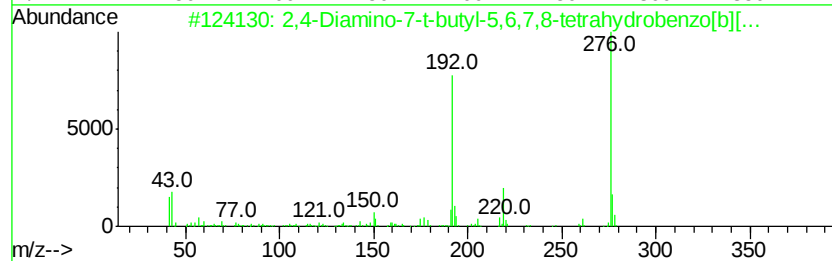
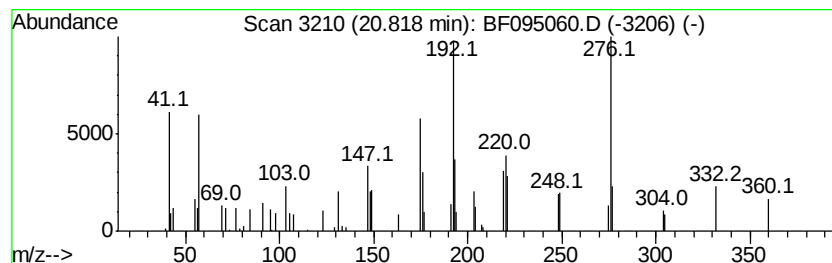
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown20.82 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.82	2.27 ng	60674	Perylene-d12	20.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Diamino-7-t-butyl-5,6,7,8-te...	276	C14H20N4S	049620-43-1	46		
2	1-[1-(Hydroxy-phenyl-methyl)-6,7...	383	C23H29N04	114609-12-0	38		
3	Bicvclo[2.2.1]hept-2-ene, 2-iodo-	220	C7H9I	058426-15-6	22		
4	Phenanthro[3,2-b]furan-7,11-dion...	276	C18H12O3	020958-17-2	22		
5	2,3-Dihydroquinoxalin-2,3-dione,...	276	C14H16N2O4	1000127-85-5	18		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
Data File : BF095060.D
Acq On : 10 May 2017 17:26
Operator : SJ/MA
Sample : I3061-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VL-WWTP-002

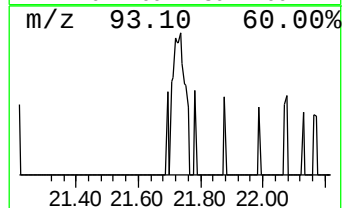
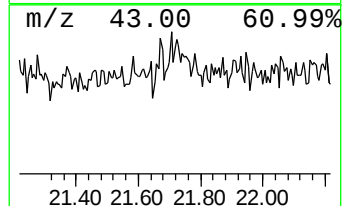
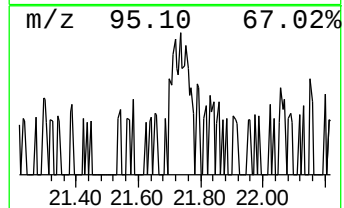
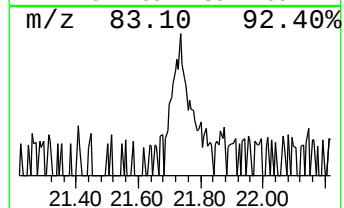
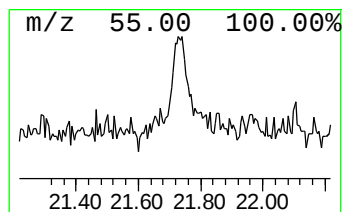
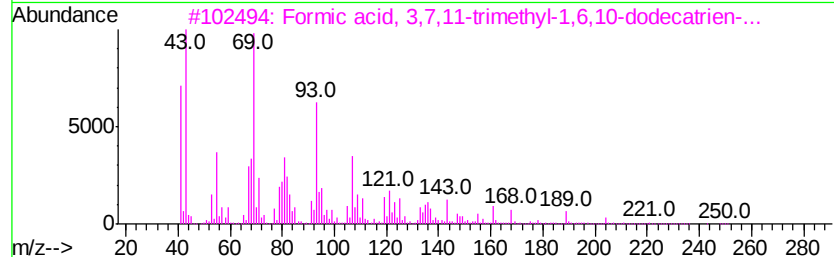
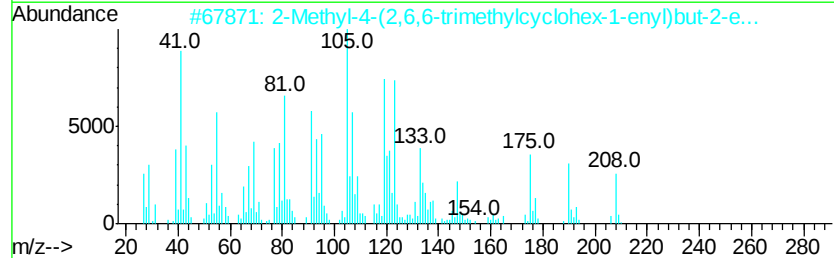
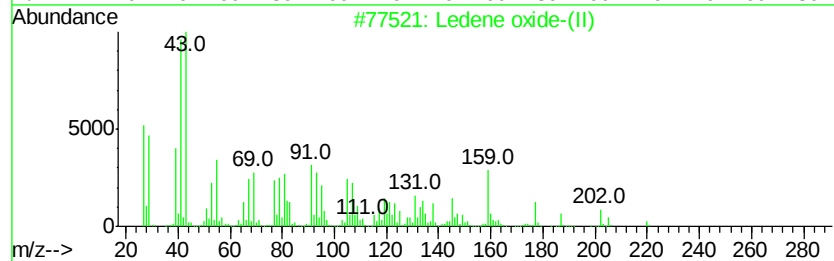
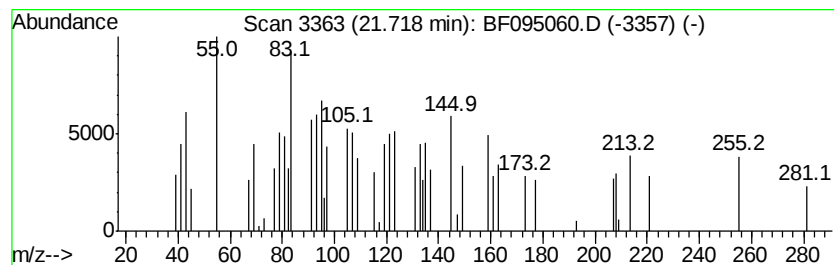
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown21.72 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	2.78 ng	74370	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ledene oxide-(II)	220	C15H24O	1000159-36-7	47
2		2-Methyl-4-(2,6,6-trimethylcyclo...	208	C14H24O	062924-17-8	35
3		Formic acid, 3,7,11-trimethyl-1,...	250	C16H26O2	1000132-11-0	22
4		Phenol, 2-(3,7-dimethylocta-2,6-...	230	C16H22O	010232-02-7	14
5		10,12-Tricosadiynoic acid, methy...	360	C24H40O2	1000333-59-4	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051017\
Data File : BF095060.D
Acq On : 10 May 2017 17:26
Operator : SJ/MA
Sample : I3061-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VL-WWTP-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.04	56.6	ng	1355150	1	7.71	478983	20.0
2-Pentanone, 4-hy...	5.00	71.5	ng	1711500	1	7.71	478983	20.0
2-Pentanone, 4-me...	6.21	16.6	ng	396572	1	7.71	478983	20.0
unknown7.37	7.37	60.8	ng	1456410	1	7.71	478983	20.0
Benzenemethanol, ...	13.55	3.4	ng	123334	3	12.56	734788	20.0
unknown13.61	13.61	3.0	ng	110173	3	12.56	734788	20.0
Octadecanoic acid	17.01	4.1	ng	158825	5	18.63	767174	20.0
unknown20.82	20.82	2.3	ng	60674	6	20.30	534800	20.0
unknown21.72	21.72	2.8	ng	74370	6	20.30	534800	20.0